Large-Scale Differential Variational Inequalities for Heterogeneous Materials:

An introduction to a new SciDAC-e project in support of the

CMSNF

Center for Materials Science of Nuclear Fuel

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Motivation: Microstructure Evolution in Materials

- **Differential Variational Inequalities (DVIs) arise in CMSNF models**
  - **Phase Field Approach:** Modeling microstructure at the mesoscale
  - Diffuse boundary between phases must be localized: use double obstacle potentials to generate free energy functional: results in a DVI
- **Challenges**
  - Lack of software for large-scale DVIs
  - Prevailing (non-DVI) approach approximates dynamics of phase variable using a smoothed potential: Stiff problem and undesirable physical artifacts
    - phase field variable does not have a compact support
    - boundary between phases is no longer localized

Vision of our SciDAC-e Project

Center for Materials Science of Nuclear Fuel

- **Broad aim: Develop advanced numerical techniques and scalable software for DVIs for the resolution of large-scale, heterogeneous materials problems**
- Collaboration among CMSNF and TOPS researchers
- **Goals**
  - Create software for resolving mesoscale models of heterogenous materials with a methodology that removes the modeling compromises that have been needed up to this point
  - Leverage emerging extreme-scale computing resources to enable simulations with billions of discretization nodes (or thousands of grains) and thus to develop a predictive capability for virtually any phenomenon of interest concerning radiation in nanostructures

Towards Optimal Petascale Simulations

PI: David Keyes, Columbia Univ.
www.scalablesolvers.org

3-Pronged Approach

- **Model heterogeneous materials with DVIs**
  - Led by M. Anitescu and A. El-Azab
  - Model phase field equations as DVIs for all classes of materials that confront CMSNF
- **Apply scalable algorithms for the resulting variational inequalities (VIs)**
  - Led by T. Munson
  - Resolve the subproblems of the time-stepping procedure using
    - Semismooth, active set, and interior-point approaches
    - Employ specialized multigrid techniques that map the active set between levels without impeding optimal convergence and scalability
- **Develop flexible, scalable VI software**
  - Led by L. C. McInnes and B. Smith
  - Build on infrastructure of PETSc and TAO (two TOPS numerical libraries)
  - Leverage work by TOPS colleagues Xiao-Chuan Cai and David Keyes in complementary SciDAC-e project, *Scalable Solvers for Fully Coupled Nuclear Fuel Modeling*

Heterogeneous Materials Modeling with DVIs

- Use a phase field model to describe microstructure:
  - Use a diffuse boundary representation for the region between phases; this may be more suitable physically for the scales used, and better handles phase disappearance. The boundary is defined by means of a phase variable $-1 \le \phi \le 1$; the interface region is the one where $-1 < \phi < 1$
  - Write a free energy functional that includes a double obstacle potential (which allows for finite boundary region extension); in turn the inequalities on the phase field variable have to be treated by hard constraints.
  - Write the dynamics of the phase configuration using the mobilities provided by the CMSNF. Due to the double obstacle potential, these have a free boundary; the resulting equations are Allen-Cahn and Cahn-Hilliard with free boundary.
  - We discretize in time, enforcing the free boundary configuration implicitly. This results in a variational inequality to be solved at each step.

DVI Formulation

- Differential Variational Inequalities
  - Arise whenever both dynmics and inequalities/switching appear in model
  - Mixture of differential equations and variational inequalities

$$
\begin{array}{rcl}
y' & = & f(t, y(t), x(t)) \\
x(t) & \in & SOL(K; F(t, y(t), \cdot)) \\
y(0) & = & y_0
\end{array}
$$

$$x \in SOL(K; F(t, y, \cdot) \Leftrightarrow (\tilde{x} - x)^T F(t, y, x) \geq 0, \forall \tilde{x} \in K$$

  - In the case of complementarity, $K = \mathbb{R}^n_+$

$$
\begin{array}{rcl}
y' & = & f(t, y(t), x(t)) \\
0 & \leq & x(t); F(t, y(t), x(t)) \\
0 & = & x(t)^T F(t, y(t), x(t)) \\
y(0) & = & y_0
\end{array}
$$

Scalable Algorithms for Variational Inequalities

- Build on capabilities in the Toolkit for Advanced Optimization (TAO)
  - www.mcs.anl.gov/tao
  - Parallel software for numerical optimization, uses PETSc for linear algebra
- Focus:
  - Semismooth methods
    - Begin with box-constrained VI: semismooth reformulation using nonlinear complimentarity problem
    - Multigrid semismooth methods
  - Active set methods
  - Interior-point methods

Semismooth Reformulation for Box-Constrained Variational Inequalities

- Nonlinear complementarity problem:

  $$o \le x \quad \perp \quad F(x) \ \ge 0,$$

  where $\perp$ implies componentwise that at the solution, either

  $$x_i = 0 \ \text{ or } \ F_i(x) = 0$$

- Reformulate using a function $\phi(\mathrm{a,b})$ with the property that

  $$\phi(\mathrm{a,b}) \ = \ 0 \quad \Leftrightarrow \quad 0 \le \mathrm{a} \ \perp \ \mathrm{b} \ge 0$$

  Fischer-Burmeister function: $\phi(\mathrm{a,b}) \ = \ \mathrm{a} + \mathrm{b} - \sqrt{\mathrm{a}^2 + b^2}$

- Thus, we solve

  $$\Phi(x, F(x)) = 0, \ \text{ where } \ \Phi_i(x, F(x)) = \phi(x_i, F_i(x))$$

  using a globalized Newton method

Scalable Software for Variational Inequalities

- Develop a new VI problem class in PETSc (www.mcs.anl.gov/petsc)
  - Develop a VI solver interface
  - Develop 3 complementary VI solver implementations based on
    - Semismooth algorithms
    - Active set methods
    - Interior point methods
- Build on SNES component of PETSc: Scalable Nonlinear Equations Solvers
  - Preconditioned Newton-Krylov methods with line search or trust region variants
  - User provides code for nonlinear function evaluation
  - User can provide code for Jacobian computation (or alternatively PETSc can compute using sparse finite differences or automatic differentiation)
  - SNES overview: see http://www.mcs.anl.gov/~curfman/docs/mcinnes-siam09.pdf
- Box-constrained VI: Require user to provide bounds on variables for SNES; otherwise, interface will remain largely unchanged

Modeling Issues Specific to CMSNF Applications

- Issues in adopting phase field approach to model microstructure evolution under irradiation conditions
  - Selection of phase field variables and representation of free energy functional in terms of these variables
  - Explicit representation of radiation environment into phase field kinetic equations
- Test cases
  - Single-void dynamics in UO_2
  - Multiple-void dynamics in UO_2
  - Nucleation and growth of void ensembles

Personnel Update

- New hire:
  - Lei Wang, Ph.D. in Applied and Interdisciplinary Mathematics from the University of Michigan, May 2010
  - Will begin working at Argonne on Sept 20, 2010
  - Focusing on modeling, with M. Anitescu and A. El-Azab
- In the process of interviewing candidates for algorithms/ software postdoc position
- Support for 2 graduate students during summer 2011
- Possibly other student/faculty/research visitors also